

Diethylmalonic acid, dodecyl hexyl ester

Inchi:	InChI=1S/C25H48O4/c1-5-9-11-13-14-15-16-17-18-20-22-29-24(27)25(7-3,8-4)23(26)28
InchiKey:	JKBMNBGLJQOXPB-UHFFFAOYSA-N
Formula:	C25H48O4
SMILES:	CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCCCC
Mol. weight [g/mol]:	412.65

Physical Properties

Property code	Value	Unit	Source
gf	-305.38	kJ/mol	Joback Method
hf	-1057.68	kJ/mol	Joback Method
hfus	58.67	kJ/mol	Joback Method
hvap	88.26	kJ/mol	Joback Method
log10ws	-7.77		Crippen Method
logp	7.380		Crippen Method
mcvol	377.990	ml/mol	McGowan Method
pc	813.07	kPa	Joback Method
rinpol	2557.00		NIST Webbook
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tb	920.75	K	Joback Method
tc	1128.53	K	Joback Method
tf	518.25	K	Joback Method
vc	1.472	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1281.05	J/molxK	920.75	Joback Method
cpg	1301.43	J/molxK	955.38	Joback Method
cpg	1320.39	J/molxK	990.01	Joback Method
cpg	1338.00	J/molxK	1024.64	Joback Method
cpg	1354.32	J/molxK	1059.27	Joback Method
cpg	1369.40	J/molxK	1093.90	Joback Method
cpg	1383.30	J/molxK	1128.53	Joback Method
dvisc	0.0004198	Paxs	518.25	Joback Method

dvisc	0.0001876	Paxs	585.33	Joback Method
dvisc	0.0000990	Paxs	652.42	Joback Method
dvisc	0.0000588	Paxs	719.50	Joback Method
dvisc	0.0000382	Paxs	786.58	Joback Method
dvisc	0.0000265	Paxs	853.67	Joback Method
dvisc	0.0000195	Paxs	920.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369447&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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